Table of contents, Volume 31, 2005

Abs-Wurmbach I → Taran MN
Ahsbahs H → Sowa H
Akaogi M, Kamii N, Kishi A, Kojitani H: Calorimetric study on high-pressure transitions in $KAlSi_3O_8$ 85
Alba MD, Castro MA, Naranjo M, Perdigón AC: Structural localization of Al^{3+} ions in aluminosilicates: application of heteronuclear chemical shift correlation to 2:1 phyllosilicates 195
Alfredsson M, Brodholt JP, Dobson DP, Oganov AR, Catlow CRA, Parker SC, Price GD: Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite 671
Alimpiev AI → Solntsev VP
Allen GC → Black L
Alp EE → Shen G
Amos TG → Majzlan J
Amthauer G → Di Benedetto F
Angel RJ → Zhao J
Arpe J → Saragovi C
Artacho E → Craig MS
Auzende A-L, Daniel I, Reynard B, Lemaire C, Guyot F: High-pressure behaviour of serpentine minerals: a Raman spectroscopic study 269

Bajda T → Mozgawa W
Barrero CA → Saragovi C
Becker KD → Ullrich K
Bente K → Huber AL
Bermanec V → da Costa GM
Bernardini GP, Borgheresi M, Cipriani C, Di Benedetto F, Romanelli M: Mn distribution in sphalerite: an EPR study 80
Bernardini GP → Di Benedetto F
Black L, Garbev K, Stemmermann P, Hallam KR, Allen GC: X-ray photoelectron study of oxygen bonding in crystalline C–S–H phases 337
Blanchard M, Ingrin J: Hydrogen diffusion in Dora Maira pyrope 593
Bläß UW, Langenhorst F, Boffa-Ballaran T, Seifert F, Frost DJ, McCammon CA: A new oxygen-deficient perovskite phase $Ca(Fe_{0.4}Si_{0.6})O_{2.8}$ and phase relations along the join $CaSiO_3$–$CaFeO_{2.5}$ at transition zone conditions 52
Boerio-Goates J → Majzlan J
Boffa-Ballaran T → Gatta GD
Boffa-Ballaran T → Rodehorst U
Boffa-Ballaran T → Bläß UW
Borgheresi M → Bernardini GP
Borrini D → Di Benedetto F
Boscherini F → Quartieri S
Bosenick A → Malcherek T
Botella V, Timon V, Escamilla-Roa E, Hernández-laguna A, Sainz-Díaz CI: Hydrogen bonding and vibrational properties of hydroxy groups in the crystal lattice of dioctahedral clay minerals by means of first principles calculations 475
Bourova E, Parker SC, Richet P: High-temperature structure and dynamics of coesite (SiO_2) from numerical simulations 569
Brodholt JP → Alfredsson M
Bromiley GD → Huber AL
Buchet R → Petit S
Burns PC → Majzlan J

Cámara F → Iezzi G
Caneschi A, Cipriani C, Di Benedetto F, Sessoli R: Characterisation of the antiferromagnetic transition of Cu_2FeSnS_4, the synthetic analogue of stannite 190
Caracas R, Gonze X: High-pressure isosymmetrical phase transition in calaverite 553
Carpenter MA → Rodehorst U
Castro MA → Alba MD
Catlow CRA → Alfredsson M
Chen J → Liu H
Churakov SV, Wunder B: Ab-initio calculations of the proton location in topaz-OH, $Al_2SiO_4(OH)_2$ 131
Cipriani C → Bernardini GP
Cipriani C → Caneschi A
Císařová I → Skála R
Claridge RFC → Tennant WC
Comodi P → Gatta GD
Cooke DJ, Redfern SE, Parrer SC: Atomistic simulation of the structure and segregation to the (0001) and (0112) surfaces of Fe_2O_3
Cox DF → Gibbs GV
Craig MS, Warren MC, Dove MT, Gale JD, Sanchez-Portal D, Ordejon P, Soler JM, Artacho E: Simulations of minerals using density-functional theory based on atomic orbitals for linear scaling 12
Crawford MK → Majzlan J

da Costa GM, Scholz R, Karfunkel J, Bermanec V, de Sá Carneiro Chaves ML: ^{57}Fe-Mössbauer spectroscopy on natural eosphorite-childrenite-ernstite samples 714
D'Acapito F → Quartieri S
Dalconi MC → Quartieri S
Daniel I → Auzende A-L
Daniel P → Zhang M
Dapiaggi M → Levy D
de Sá Carneiro Chaves ML → da Costa GM
Decarreau A → Petit S
Della Giusta A → Lavina B
Della Ventura G → Iezzi G
Delwiche J → Hatert F
Di Benedetto F, Bernardini GP, Borrini D, Lottermoser W, Tippelt G, Amthauer G: ^{57}Fe– and ^{119}Sn–Mössbauer study on stannite (Cu_2FeSnS_4)-kesterite (Cu_2ZnSnS_4) solid solution 683
Di Benedetto F → Bernardini GP
Di Benedetto F → Caneschi A
Di Vincenzo G → Viti C
Diella V → Levy D
Dobson DP → Alfredsson M
Dove MT → Craig MS
Dovesi R → Prencipe M

E Redfern S → J Cooke D
Escamilla-Roa E → Botella V
Ewing RC → Zhang M

Fehr KT → Huber AL
Fernandes Scalvi RM, Li MS, Scalvi LVA: Thermal annealing-induced electric dipole relaxation in natural alexandrite 733
Fransolet A-M → Hatert F
Frost D → Taran MN
Frost DJ → Bläß UW
Fukuoka K → Shimoda K
Funakoshi K → Nishihara Y

Gaft M, Nagli L, Waychunas G, Weiss D: The nature of blue luminescence from natural benitoite $BaTiSi_3O_9$ 365
Gale JD → Craig MS
Garbev K → Black L
Gatta GD, Boffa-Ballaran T, Comodi P, Zanazzi PF: Comparative compressibility and equation of state of orthorhombic and tetragonal edingtonite 288
Gatta GD, Wells SA: Rigid unit modes at high pressure: an explorative study of a fibrous zeolite-like framework

with EDI topology 465
Geiger CA → Rodehorst U
Geiger CA → Kolesov BA
Geisler T → Zhang M
Gemmi M → Levy D
Gerya TV, Podlesskii KK, Perchuk LL, Maresch WV: Semi-empirical Gibbs free energy formulations for minerals and fluids for use in thermodynamic databases of petrological interest 429
Gibbs GV, Cox DF, Ross NL: A modeling of the structure and favorable H-docking sites and defects for the high-pressure silica polymorph stishovite 232
Gonze X → Caracas R
Grandjean F → Hatert F
Guedes KJ → Krambrock K
Guyot F → Auzende A-L

Hålenius U → Lenaz D
Hallam KR → Black L
Hamaya N → Okada T
Harlov DE → Mookherjee M
Hatert F, Long GJ, Hautot D, Fransolet A-M, Delwiche J, Hubin-Franskin MJ, Grandjean F: A structural, magnetic, and Mössbauer spectral study of several Na–Mn–Fe-bearing alluaudites 487
Haussühl S, Liebertz J: Elastic and thermoelastic properties of synthetic $Ca_2MgSi_2O_7$ (åkermanite) and $Ca_2ZnSi_2O_7$ (hardystonite) 565
Hautot D → Hatert F
Hernández-laguna A → Botella V
Heuer M → Huber AL
Heyroth F → van Aken PA
Hirao N, Ohtani E, Kondo T, Kikegawa T: Equation of state of iron–silicon alloys to megabar pressure 329
Höche T → van Aken PA
Holl CM → Smyth JR
Hriljac JA → Lee Y
Hu J → Liu H
Huber AL, Heuer M, Fehr KT, Bente K, Schmidbauer E, Bromiley GD: Characterization of synthetic hedenbergite ($CaFeSi_2O_6$)–petedunnite ($CaZnSi_2O_6$) solid solution series by X-ray powder diffraction and ^{57}Fe Mössbauer spectroscopy 67
Hubin-Franskin MJ → Hatert F

Iezzi G, Cámara F, Della Ventura G, Oberti R, Pedrazzi G, Robert J-L: Synthesis, crystal structure and crystal chemistry of ferri-clinoholmquistite, $\square Li_2Mg_3Fe^{3+}{}_2Si_8O_{22}(OH)_2$ 375
Iguchi T → Nishihara Y
Ingrin J → Blanchard M
Islam MS → Jones A

Javorský P → Thiriet C
Jiménez de Haro MC → Pérez-Rodríguez JL
Johnson EA, Rossman GR: An infrared and ^1H MAS NMR investigation of strong hydrogen bonding in ussingite, $Na_2AlSi_3O_8(OH)$ 115
Jones A, Islam MS, Mortimer M, Palmer D: Alkali ion migration in albite and K-feldspar 313

Kamada T → Kudoh Y
Kameda J → Saruwatari K
Kamii N → Akaogi M
Kaneko H → Okada T
Karfunkel J → da Costa GM
Katayama S → Shimoda K
Kawamoto T → Matsukage KN
Kawamoto T → Smyth JR
Keding R → van Aken PA
Kikegawa T → Hirao N
Kikegawa T → Matsukage KN
Kikuchi M → Shimoda K
Kishi A → Akaogi M
Kleppe A → Smyth JR
Knight KS → Schofield PF
Koch M → Kontny A
Kojitani H → Akaogi M
Kolesov BA, Geiger CA: A Raman spectroscopic study of Fe–Mg olivines 142
Kolesov BA, Geiger CA: A temperature-dependent single-crystal Raman spectroscopic study of fayalite: evidence for phonon-magnetic excitation coupling 155
Kondo T → Hirao N
Konings RJM → Thiriet C
Kontny A, Woodland AB, Koch M: Temperature-dependent magnetic susceptibility behaviour of spinelloid and spinel solid solutions in the systems Fe_2SiO_4–Fe_3O_4 and $(Fe,Mg)_2SiO_4$–Fe_3O_4 28
Koyano M → Shimoda K
Krambrock K, Pinheiro MVB, Guedes KJ, Medeiros SM, Schweizer S, Spaeth J-M: Correlation of irradiation-induced yellow color with the O^- hole center in tourmaline 168
Kubo T, Shimojuku A, Ohtani E: Mg–Fe interdiffusion rates in wadsleyite and the diffusivity jump at the 410-km discontinuity 456
Kudoh Y, Kuribayashi T, Suzuki A, Ohtani E, Kamada T: Space group and hydrogen sites of δ-AlOOH and implications for a hypothetical high-pressure form of $Mg(OH)_2$ 360
Kunzmann Th → Schmidbauer E
Kuribayashi T → Kudoh Y

Langenhorst F → Bläß UW
Langenhorst F → Smyth JR
Langer K → Ullrich K
Langer K → Taran MN
Laustsen HMS → Smyth JR
Lavina B, Salviulo G, Della Giusta A: Structure modelling and cation partitioning of spinel solid solutions at high T,P conditions 45
Lee Y, Hriljac JA, Studer A, Vogt T: Anisotropic compression of edingtonite and thomsonite to 6 GPa at room temperature 22
Lee Y, Hriljac JA, Vogt T: Pressure-induced migration of zeolitic water in laumontite 421
Lees NS → Tennant WC
Lemaire C → Auzende A-L
Lenaz D, Skogby H, Princivalle F, Hålenius U: Structural changes and valence states in the $MgCr_2O_4$–Fe-Cr_2O_4 solid solution series 633
Lerf A → Pérez-Rodríguez JL
Levy D, Diella V, Dapiaggi M, Sani A, Gemmi M, Pavese A: Equation of state, structural behaviour and phase diagram of synthetic $MgFe_2O_4$, as a function of pressure and temperature 122
Li MS → Fernandes Scalvi RM
Liebertz J → Haussühl S
Likhacheva AYu, Veniaminov SA, Paukshtis EA: Thermal decomposition of NH_4-analcime 306
Liu H, Hu J, Xu J, Liu Z, Shu J, Mao HK, Chen J: Phase transition and compression behavior of gibbsite under high-pressure 240
Liu Z → Liu H
Long GJ → Hatert F
Lottermoser W → Di Benedetto F

Maekawa H → Nakatsuka A
Majzlan J, Stevens R, Boerio-Goates J, Woodfield BF, Navrotsky A, Burns PC, Crawford MK, Amos TG: Thermodynamic properties, low-temperature heat-capacity anomalies, and single-crystal X-ray refinement of hydronium jarosite, $(H_3O)Fe_3(SO_4)_2(OH)_6$ 518
Malcherek T, Bosenick A: Structure and phase transition of $CaGe_2O_5$ revisited 224
Mao HK → Liu H
Mao H-R → Shen G
Maresch WV → Gerya TV
Martin F → Petit S
Mashkovtsev RI → Solntsev VP
Matsukage KN, Ono S, Kawamoto T, Kikegawa T: The compressibility of a natural apatite 580
McCammon CA → Bläß UW
McCammon CA → Smyth JR
Medeiros SM → Krambrock K
Mellini M → Viti C
Meng Y → Shen G
Mizota T → Nakatsuka A
Mookherjee M, Redfern S, Swainson I, Harlov DE: Low-temperature

behaviour of ammonium ion in buddingtonite $[N(D/H)_4AlSi_3O_8]$ from neutron powder diffraction 643
Mortimer M → Jones A
Mozgawa W, Bajda T: Spectroscopic study of heavy metals sorption on clinoptilolite 706

Nagli L → Gaft M
Nakashima S → Okumura S
Nakatsuka A, Ueno H, Nakayama N, Mizota T, Maekawa H: Single-crystal X-ray diffraction study of cation distribution in $MgAl_2O_4$–$MgFe_2O_4$ spinel solid solution 278
Nakayama K → Nishihara Y
Nakayama N → Nakatsuka A
Naranjo M → Alba MD
Navrotsky A → Majzlan J
Nishihara Y, Nakayama K, Takahashi E, Iguchi T, Funakoshi K: *P-V-T* equation of state of stishovite to the mantle transition zone conditions 660

Oberti R → Iezzi G
Oberti R → Quartieri S
Oganov AR → Alfredsson M
Ohtani E → Hirao N
Ohtani E → Kudoh Y
Ohtani E → Kubo T
Okada T, Utsumi W, Kaneko H, Turkevich V, Hamaya N, Shimomura O: Kinetics of the graphite–diamond transformation in aqueous fluid determined by in-situ X-ray diffractions at high pressures and temperatures 261
Okumura S, Nakashima S: Water diffusivity in rhyolitic glasses as determined by in situ IR spectroscopy 183
Okuno M → Shimoda K
Ono S → Matsukage KN
Ordejon P → Craig MS
Orlando R → Prencipe M
Ott O → Ullrich K

Palmer D → Jones A
Parker SC → Cooke DJ
Parker SC → Bourova E
Parker SC → Alfredsson M
Pascale F → Prencipe M
Paukshtis EA → Likhacheva AYu
Pavese A → Levy D
Pedrazzi G → Iezzi G
Perchuk LL → Gerya TV
Perdigón AC → Alba MD
Pérez-MaquedaLA→Pérez-RodríguezJL
Pérez-Rodríguez JL, Poyato J, Jiménez de Haro MC, Pérez-Maqueda LA, Lerf A: Thermal decomposition of NH_4^+-vermiculite from Santa Olalla (Huelva, Spain) and its relation to the metal ion distribution in the octahedral sheet 415
Petit S, Decarreau A, Martin F, Buchet R: Refined relationship between the position of the fundamental OH stretching and the first overtones for clays 585
Pinheiro MVB → Krambrock K
Platonov AN → Taran MN
Podlesskii KK → Gerya TV
Poyato J → Pérez-Rodríguez JL
Prakapenka VB → Shen G
Prencipe M, Pascale F, Zicovich-Wilson CM, Saunders VR, Orlando R, Dovesi R: The vibrational spectrum of calcite ($CaCO_3$): an ab initio quantum-mechanical calculation 559
Price GD → Alfredsson M
Princivalle F → Lenaz D

Quartieri S, Dalconi MC, Boscherini F, Oberti R, D'Acapito F: Changes in the local coordination of trace rare-earth elements in garnets by high-energy XAFS: new data on dysprosium 162

Redfern S → Mookherjee M
Redfern SE → Cooke DJ
Reynard B → Auzende A-L
Richet P → Bourova E
Robert J-L → Iezzi G
Rodehorst U, Carpenter MA, Boffa Ballaran T, Geiger CA: Local structural heterogeneity, mixing behaviour and saturation effects in the grossular–spessartine solid solution 387
Romanelli M → Bernardini GP
Ross NL → Zhao J
Ross NL → Gibbs GV
Rossman GR → Smyth JR
Rossman GR → Johnson EA

Sainz-Díaz CI → Botella V
Salje EKH → Zhang M
Salviulo G → Lavina B
Sanchez LC → Saragovi C
Sanchez-Portal D → Craig MS
Sani A → Levy D
Saragovi C, Arpe J, Sileo E, Zysler R, Sanchez LC, Barrero CA: Changes in the structural and magnetic properties of Ni-substituted hematite prepared from metal oxinates 625
Saruwatari K, Kameda J, Tanaka H: Generation of hydrogen ions and hydrogen gas in quartz–water crushing experiments: an example of chemical processes in active faults 176
Saunders VR → Prencipe M
Scalvi LVA → Fernandes Scalvi RM
Schmidbauer E, Kunzmann Th: Electrical conductivity, thermopower and ^{57}Fe Mössbauer spectroscopy of aegirine ($NaFeSi_2O_6$) 102
Schmidbauer E → Huber AL
Schmitz W → Sowa H
Schofield PF, Knight KS, van der Houwen JAM, Valsami-Jones E: The role of hydrogen bonding in the thermal expansion and dehydration of brushite, Di-calcium phosphate dihydrate 606
Scholz R → da Costa GM
Schweizer S → Krambrock K
Seifert F → Bläß UW
Sessoli R → Caneschi A
Shen G, Sturhahn W, Alp EE, Zhao J, Toellner TS, Prakapenka VB, Meng Y, Mao H-R: Phonon density of states in iron at high pressures and high temperatures 353
Shimoda K, Okuno M, Syono Y, Kikuchi M, Fukuoka K, Koyano M, Katayama S: Structural evolutions of an obsidian and its fused glass by shock-wave compression 532
Shimojuku A → Kubo T
Shimomura O → Okada T
Shu J → Liu H
Sileo E → Saragovi C
Skála R, Císařová I: Crystal structure of meteoritic schreibersites: determination of absolute structure 721
Skogby H → Lenaz D
Smyth JR, Holl CM, Langenhorst F, Laustsen HMS, Rossman GR, Kleppe A, McCammon CA, Kawamoto T, van Aken PA: Crystal chemistry of wadsleyite II and water in the Earth's interior 691
Soler JM → Craig MS
Solntsev VP, Tsvetkov EG, Alimpiev AI, Mashkovtsev RI: Valent state and coordination of cobalt Ions in beryl and chrysoberyl crystals 1
Sowa H, Ahsbahs H, Schmitz W: X-ray diffraction studies of millerite NiS under non-ambient conditions 321
Spaeth J-M → Krambrock K
Stemmermann P → Black L
Stevens R → Majzlan J
Studer A → Lee Y
Sturhahn W → Shen G
Suzuki A → Kudoh Y
Swainson I → Mookherjee M
Syono Y → Shimoda K

Takahashi E → Nishihara Y
Tanaka H → Saruwatari K
Taran MN, Langer K, Abs-Wurmbach I, Frost D, Platonov AN: Local relaxation around $^{[6]}Cr^{3+}$ in synthetic pyrope–knorringite garnets, $^{[8]}Mg_3{}^{[6]}(Al_{1-X}\,Cr_X{}^{3+})_2{}^{[4]}Si_3O_{12}$, from electronic absorption spectra 650
Tennant WC, Claridge RFC, Walsby CJ, Lees NS: Point defects in crystalline zircon (zirconium silicate), $ZrSiO_4$: electron paramagnetic resonance studies 203

Thiriet C, Konings RJM, Javorský P, Wastin F: The heat capacity of cerium orthophosphate $CePO_4$, the synthetic analogue of monazite 347
Timon V → Botella V
Tippelt G → Di Benedetto F
Toellner TS → Shen G
Tossell JA: Calculation of ^{17}O NMR shieldings in molecular models for crystalline MO, M = Mg, Ca, Sr, and in models for alkaline earth silicates 41
Tsvetkov EG → Solntsev VP
Turkevich V → Okada T

Uecker R → van Aken PA
Ueno H → Nakatsuka A
Ullrich K, Ott O, Langer K, Becker KD: Temperature dependence of the polarized electronic absorption spectra of olivines. Part II—Cobalt-containing olivines 247
Utsumi W → Okada T

Valsami-Jones E → Schofield PF
van Aken PA, Höche T, Heyroth F, Keding R, Uecker R: Insights into oxygen-cation bonding in fresnoite-type structures from O *K*- and Ti L_{23}- electron energy-loss spectra and abinitio calculations of the electronic structure 543
van Aken PA → Smyth JR
van der Houwen JAM → Schofield PF
Veniaminov SA → Likhacheva AYu
Viti C, Di Vincenzo G, Mellini M: Thermal transformations in laser-heated chloritized annite 92
Vogt T → Lee Y

Walsby CJ → Tennant WC
Warren MC → Craig MS
Wastin F → Thiriet C
Waychunas G → Gaft M
Weiss D → Gaft M
Wells SA → Gatta GD
Woodfield BF → Majzlan J
Woodland AB → Kontny A
Wunder B → Churakov SV

Xu J → Liu H

Zanazzi PF → Gatta GD
Zanazzi PF → Gatta GD 288
Zhang M, Salje EKH, Ewing RC, Daniel P, Geisler T: Applications of near-infrared FT-Raman spectroscopy in metamict and annealed zircon: oxidation state of U ions 405
Zhao J, Ross NL, Angel RJ: Tilting and distortion of $CaSnO_3$ perovskite to 7 GPa determined from single-crystal X-ray diffraction 299
Zhao J → Shen G
Zicovich-Wilson CM → Prencipe M
Zysler R → Saragovi C